ENSLAPP-A-546/95, hep-ph/9509302

The dynamics of a thermal non-equilibrium anharmonic oscillator

Herbert Nachbagauer ‡
*Laboratoire de Physique Théorique ENSLAPP * Chemin de Bellevue, BP 110, F - 74941 Annecy-le-Vieux Cedex, France*
(February 1, 2008)

Abstract

We propose an non-standard method to calculate non-equilibrium physical observables. Considering the generic example of an anharmonic quantum oscillator, we take advantage of the fact that the commutator algebra of second order polynomials in creation/annihilation operators closes. We solve the von Neumann equation for the density-operator exactly in the mean field approximation and study the time evolution of the particle number and the expectation value $\langle X^2 \rangle$.

11.10.Wx, 05.30.-d

‡e-mail: herby @ lapphp1.in2p3.fr

*URA 14-36 du CNRS, associée à l'E.N.S. de Lyon, et au L.A.P.P. (IN2P3-CNRS) d'Annecy-le-Vieux

INTRODUCTION

The consistent calculation of equilibrium finite-temperature physical observables requires a resummation of the leading temperature contributions along the lines of the Braaten-Pisarski [1] resummation program established already some years ago. The application of those ideas to scalar theories, QED, QCD and the electroweak model has been extremely successful so far, although the original resummation may have to be modified slightly near the light-cone for models involving massless particles. On the other hand, many interesting realistic physical scenarios like, e.g., phase transitions [2] and particle production in a plasma are clearly out-of-equilibrium or only nearly-equilibrium systems in which case the field theoretical framework lacks a systematic basis and the straight-forward application of basically linear response methods gives rise to potential inconsistencies, such as pinch singularities [3]. In this note we consider the toy-model of a quantum-mechanically anharmonic oscillator which can be solved exactly.

THE THERMAL ANHARMONIC OSCILLATOR

The model under consideration is characterized by the Hamiltonian

$$H = H_0 + H_I, \quad H_0 = \frac{1}{2}P^2 + \frac{\omega^2}{2}X^2, \quad H_I = \frac{\lambda\omega^3}{2}X^4, \tag{1}$$

the quartic interaction-therm mimicking a self-interaction term as in the field-theoretical analog. Since there quadratic Hamiltonians are the only ones which can be integrated out exactly, we will also here focus on the so-called mean-field approximation. The basic idea is to expand the Hamiltonian operator around an expectation value that at finite temperature T (and for mixed states in general) is given by the trace of the product of the corresponding operator with the normalized density-operator of the state. For the Hamiltonian above being parity even, the natural expansion parameter is $\delta X^2 = X^2 - \langle X^2\rangle$. Dropping the $(\delta X^2)^2$ term, the quadratic contribution of the interaction Hamiltonian, $H_I^{quadr.} = {}^1\!/_2\lambda\omega^3\langle X^2\rangle(2X^2 - \langle X^2\rangle)$, has a form analogous to H_0 with time-dependent frequency. In terms of creation and annihilation operators, $a = \sqrt{2\omega}X + \mathrm{i}\sqrt{2/\omega}P$ and $a^\dagger$, the effective free Hamiltonian $H^{quadr.}$ under study is thus composed of

$$H_I^{quadr.} = \frac{\lambda\omega}{2}f(t)(a^{\dagger 2} + 2a^\dagger a + a^2 + \mathbf{1} - f(t)) \quad \text{and} \quad H_0 = \omega(a^\dagger a + \frac{1}{2}) \tag{2}$$

where $f(t)/\omega = \langle X^2\rangle = Z^{-1}\,\mathrm{Tr}(\rho X^2)$ has to be determined self-consistently. Note that diagonalizing the quadratic Hamiltonian would render the vacuum definition $a\,|0\rangle = 0$ time dependent.

The density operator for the system in thermal equilibrium

$$\rho_{eq} = Z_{eq}^{-1}\exp(-H/T), \quad Z_{eq} = \mathrm{Tr}(\rho_{eq}), \tag{3}$$

which minimizes the equilibrium entropy functional $S \sim \mathrm{Tr}(\rho\log\rho)$, is a particular solution of the von Neumann equation of motion

$$i\frac{\mathrm{d}}{\mathrm{d}t}\rho = [H, \rho]\,. \tag{4}$$

Solutions of that equation do not uniquely determine the density-operator but admit in general additive static solutions that are functionals of eventual constants of motion. I want to point out that the equilibrium entropy functional remains constant in time for every solution of (4). For simple, e.g. zero-dimensional integrable or infinite dimensional non-interacting, systems it is argued that thermodynamic information loss has to be induced by a second averaging procedure, e.g. coarse graining in phase space [4] or in temperature [5], or time smoothing. For more complicated systems as quantum field-theoretical models or classical many-body systems the second averaging process is hidden in asymptotic approximations, and particularly in cutting the Bogoliubov-Born-Green-Kirkwood-Yvon hierarchies [6], generally resulting in a kinetic equation. We want to mention that besides those somehow artificial and pragmatic methods there exists, based on a couple of evident assumptions, a systematic approach to clearly distinguish thermodynamic (the 'relevant') and microdynamic (the 'irrelevant') part of the dynamics [7] which, however, has not yet been applied systematically within the framework of quantum field-theory so far. We will not address these open questions further but pursue the modest task to find a solution of the von Neumann equation.

The biquadratic form of (2) in $a, a^\dagger$ suggests the solution ρ

$$\rho = Z^{-1}\exp(Ba^{\dagger 2})\exp(A\; a^\dagger a + g\mathbf{1})\exp(\bar{B}a^2), \quad Z = \mathrm{Tr}\rho, \tag{5}$$

where A, B and g are time dependent functions to be determined, and the hermiticity of the density operator $\rho = \rho^\dagger$ necessitates A, g real. On account of the basic relation $\left[a, a^\dagger\right] = \mathbf{1}$ the set of operators $\mathcal{S} = \left\{\mathbf{1}, a^\dagger a, a^2, a^{\dagger 2}\right\}$ forms a closed commutator algebra

$$\left[a^{\dagger 2}, a^2\right] = -2(\mathbf{1} + 2a^\dagger a) \quad \left[a^{\dagger 2}, a^\dagger a\right] = -2a^{\dagger 2} \quad \left[a^2, a^\dagger a\right] = 2a^2 \tag{6}$$

which is the essential property that allows the evaluation of the expectation values in what follows. Using relations such as

$$\mathrm{e}^{Ba^{\dagger 2}} a^2 \mathrm{e}^{-Ba^{\dagger 2}} = a^2 - 2B(\mathbf{1} + 2a^\dagger a) + 4B^2 a^{\dagger 2}$$

it is elementary algebra to commutate the summands of H to the r.h.s. of (4) and to compare with their counterparts in the time derivative. In the resulting system of ordinary first order differential equations ($B = x + \mathrm{i}y$),

$$\dot{A} = 2\dot{g} = 4\lambda f y \tag{7}$$

$$\dot{x} = 2y(1 + \lambda f) + 4\lambda f x y \tag{8}$$

$$-\dot{y} = 2x(1 + \lambda f) + 2\lambda f(x^2 - y^2) + \lambda(1 - \mathrm{e}^{2A})/2 \tag{9}$$

where the dot denotes differentiation with respect to the dimensionless time scale $\tau = \omega t$, one only needs to express $f(t)$ in terms of A, x, y. For this purpose, it is useful to study the averaged elements of $\mathcal{S}$ and to commutate $a, a^\dagger$ through ρ. Using the cyclicity of the trace, this leads to a linear system of equations for the corresponding averages with the solution

$$n = \frac{1}{Z}\mathrm{Tr}(\rho a^\dagger a) = \frac{(4r^2 + \mathrm{e}^A - \mathrm{e}^{2A})}{N}, \quad \frac{1}{Z}\mathrm{Tr}(\rho a^2) = \frac{2(x + \mathrm{i}y)}{N} \tag{10}$$

where $r^2 = x^2 + y^2$, $N = (1 - \mathrm{e}^A)^2 - 4r^2$, thus $f(t) = (1 - \mathrm{e}^{2A} + 4r^2 + 4x)/(2N)$.

The system (7-9) can be solved exactly. An integral of motion can be obtained by forming $\dot{x}x + \dot{y}y$ and eliminating f by means of (7),

$$r^2 = \frac{1}{4}(1 + \mathrm{e}^{2A} + C\mathrm{e}^A), \tag{11}$$

with an integration constant C. A second integral arises from eliminating y

$$\left(\mathrm{e}^{-A}(x + \frac{1}{2}) + \frac{C}{4}\right)^2 = \frac{C+2}{2\lambda}\mathrm{e}^{-A} + D, \tag{12}$$

with a second constant of motion D. Finally, rescaling the thermal average by $z = -f(C + 2)/2$, the time evolution is governed by the first order differential equation

$$\dot{z} = \sqrt{P(z)}, \quad P(z) = 1 - \frac{C^2}{4} + 2Cz - 4z^2 + \frac{8\lambda z}{C+2}\left(z^2 - D\right) \tag{13}$$

which may be solved in terms of Jacobi integrals. Note that the solution of $P(z) = 0$ determines the static limit of the average $\langle X^2 \rangle$.

The physical content of (13) may best be displayed by choosing particular initial conditions. Consider, e.g., that at $t = 0$ the system be prepared in the non-self-interacting ($\lambda = 0$) equilibrium state, to wit $A(0) = A_0 = -\omega/T$, $x(0) = y(0) = 0$, corresponding to the constants of motion

$$C_0 = -(\mathrm{e}^{A_0} + \mathrm{e}^{-A_0}), \quad D_0 = \frac{(1 - \mathrm{e}^{-A_0})^2}{16\lambda}\left(8 + \lambda(1 + \mathrm{e}^{A_0})^2\right). \tag{14}$$

In that case

$$f(t) = \frac{1}{2(1 - \mathrm{e}^{A_0})^2}\left(1 - \mathrm{e}^{2A_0} - u_- \,\mathrm{sn}^2(2\Omega t|m)\right) \tag{15}$$

where sn is the Jacobian Elliptic Function [8] with

$$\Omega = \sqrt{\frac{\lambda u_+}{8}}\frac{\omega}{(1 - \mathrm{e}^{A_0})} \tag{16}$$

and module $m = u_-/u_+$ where

$$u_\pm = \frac{(1 - \mathrm{e}^{A_0})}{2\lambda}\Big(2(1 - \mathrm{e}^{A_0}) + 3\lambda(1 + \mathrm{e}^{A_0}) \pm \sqrt{4(1 - \mathrm{e}^{A_0})^2 + 12\lambda(1 - \mathrm{e}^{2A_0}) + \lambda^2(1 + \mathrm{e}^{A_0})^2}\Big). \tag{17}$$

The expectation value $f(t)$ performs an anharmonic oscillation with period $\mathcal{P} = K(m)/\Omega$ where $K(m)$ is the Complete Elliptic Integral of the first kind [8]. We observe that also the occupation number corresponding to H_0 varies in time,

$$n = n_0 + \frac{\lambda u_-}{8(1-\mathrm{e}^{A_0})^4}\left(2(1-\mathrm{e}^{2A_0}) - u_-\mathrm{sn}^2(2\Omega t|m)\right)\mathrm{sn}^2(2\Omega t|m),$$
$$n_0 = (\mathrm{e}^{-A_0}-1)^{-1}, \tag{18}$$

which is not surprising since the particle-number operator H_0/ω no more commutes with the quadratic part of H. However, in the thermal average of $H^{quadr.}$,

$$h = \left\langle H^{quadr.}\right\rangle = \omega\left(n(t) + \frac{1}{2} + \frac{\lambda}{2}f(t)^2\right), \tag{19}$$

time dependence cancels out in a non-trivial way, as it should be since we have solved the von Neuman equation exactly. In fact, the two integrals of motion (11,12) are already sufficient to determine the energy h of the anharmonic oscillator

$$h = -\frac{C}{2(C+2)} + \frac{2\lambda D}{(C+2)^2} \tag{20}$$

for arbitrary initial conditions.

It is interesting to study the high temperature limit where the period approaches

$$\omega\mathcal{P} = \sqrt{\frac{\omega\pi}{2\lambda T}}\pi\left[\Gamma(\frac{3}{4})\right]^{-2} - \sqrt{\frac{\omega\pi}{2\lambda T}}^3\left(\left[\Gamma(\frac{3}{4})\right]^{-2} + \frac{1}{2}\left[\Gamma(\frac{5}{4})\right]^{-2}\right) + \mathcal{O}(T^{-\frac{5}{2}}), \tag{21}$$

which is a valid approximation for $2\lambda T \gg \omega\pi$. The period is a non-analytic function in the coupling constant in the high temperature limit. Physically this can be understood as follows. For sufficiently high T the energy levels with $E_n \sim T$ are all occupied. In that regime the shape of the potential is dominated by the quartic part, the quadratic part being rather a perturbation of it.

SUMMARY AND CONCLUSION

We studied the dynamics of a thermal non-equilibrium anharmonic oscillator. Expanding the Hamiltonian around the temperature and time dependent expectation value $\langle X^2\rangle$, the von Neuman equation can be solved exactly for the density operator. We find that the system performs an anharmonic oscillation. Specifying the initial conditions to be the non-interacting thermal equilibrium configuration, the time evolution is studied in some detail.

The basic ingredient in the calculation is that the commutator algebra of second order polynomials in creation/annihilation operators closes. This allows to commutate operators though the density operator which, together with the cyclicity of the trace, leads to a set of linear equations. It would be interesting to extend this method to go beyond the mean-field approximation which amounts to consider fourth order polynomials.

REFERENCES

[1] E. Braaten and R. D. Pisarski, Nucl. Phys. B 337 (1990) 569.

[2] See e.g.: D. Boyanovsky, H. J. de Vega and R. Holman, *Non-equilibrium dynamics of phase transitions: From the early universe to chiral condensates*, Proceedings of the *2. Journée Cosmologie*, Observatoire de Paris, June 1994, H. J. de Vega and N. Sánchez, Editors, World Scientific, 1994.

[3] A. J. Niemi and G. W. Semenoff, Ann. Phys. (N.Y.) 152 (1984) 105; Nucl. Phys. B 230[FS] (1984) 181.
H. A. Weldon, Phys. Rev. D 45 (1992) 352.
T. Altherr and D. Seibert, Phys. Lett. B 333 (1994) 149.
P. F. Bedaque, Phys. Lett. B 344 (1995) 23.

[4] See e.g.: R. Zwanzig, in *Lectures in Theoretical Physics*, edited by W. E. Brittin, B. W. Downs and J. Downs, Interscience, New York, 1961.

[5] D. N. Zubarev, *Nonequilibrium statistical thermodynamics*, Consultants Bureau, New York, 1974.

[6] E. Calzetta and B. L. Hu, Phys. Rev. D 35 (1987) 495.

[7] R. Balescu, *Equilibrium and Nonequilibrium Statistical Mechanics*, Wiley, New York, 1975.

[8] M. Abramowitz and I. A. Stegun (eds.), *Handbook of Mathematical Functions*, Dover Publ., New York, 1965.